



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 08:24 am GMT

PDB ID : 3RBJ  
Title : Crystal Structure of the lid-mutant of Streptococcus agalactiae Sortase C1  
Authors : Khare, B.; Narayana, S.V.L.  
Deposited on : 2011-03-29  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

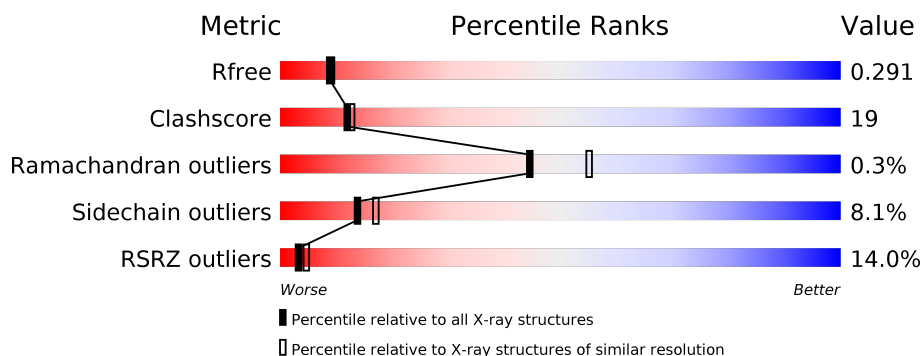
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	230	<div> <div>8%</div> <div> <div></div> <div>56%</div> <div>25%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	230	<div> <div>15%</div> <div> <div></div> <div>57%</div> <div>20%</div> <div>5%</div> <div>18%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2983 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sortase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1495	951	263	279	2			
1	B	188	Total	C	N	O	S	0	0	0
			1454	922	257	273	2			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP Q8E0S7
A	-9	ARG	-	EXPRESSION TAG	UNP Q8E0S7
A	-8	GLY	-	EXPRESSION TAG	UNP Q8E0S7
A	-7	SER	-	EXPRESSION TAG	UNP Q8E0S7
A	-6	HIS	-	EXPRESSION TAG	UNP Q8E0S7
A	-5	HIS	-	EXPRESSION TAG	UNP Q8E0S7
A	-4	HIS	-	EXPRESSION TAG	UNP Q8E0S7
A	-3	HIS	-	EXPRESSION TAG	UNP Q8E0S7
A	-2	HIS	-	EXPRESSION TAG	UNP Q8E0S7
A	-1	HIS	-	EXPRESSION TAG	UNP Q8E0S7
A	0	GLY	-	EXPRESSION TAG	UNP Q8E0S7
A	1	SER	-	EXPRESSION TAG	UNP Q8E0S7
A	48	ILE	LYS	ENGINEERED MUTATION	UNP Q8E0S7
A	49	PRO	ASP	ENGINEERED MUTATION	UNP Q8E0S7
A	50	ASN	PRO	ENGINEERED MUTATION	UNP Q8E0S7
A	51	THR	TYR	ENGINEERED MUTATION	UNP Q8E0S7
A	52	GLY	SER	ENGINEERED MUTATION	UNP Q8E0S7
A	184	ALA	CYS	ENGINEERED MUTATION	UNP Q8E0S7
B	-10	MET	-	EXPRESSION TAG	UNP Q8E0S7
B	-9	ARG	-	EXPRESSION TAG	UNP Q8E0S7
B	-8	GLY	-	EXPRESSION TAG	UNP Q8E0S7
B	-7	SER	-	EXPRESSION TAG	UNP Q8E0S7
B	-6	HIS	-	EXPRESSION TAG	UNP Q8E0S7
B	-5	HIS	-	EXPRESSION TAG	UNP Q8E0S7
B	-4	HIS	-	EXPRESSION TAG	UNP Q8E0S7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	EXPRESSION TAG	UNP Q8E0S7
B	-2	HIS	-	EXPRESSION TAG	UNP Q8E0S7
B	-1	HIS	-	EXPRESSION TAG	UNP Q8E0S7
B	0	GLY	-	EXPRESSION TAG	UNP Q8E0S7
B	1	SER	-	EXPRESSION TAG	UNP Q8E0S7
B	48	ILE	LYS	ENGINEERED MUTATION	UNP Q8E0S7
B	49	PRO	ASP	ENGINEERED MUTATION	UNP Q8E0S7
B	50	ASN	PRO	ENGINEERED MUTATION	UNP Q8E0S7
B	51	THR	TYR	ENGINEERED MUTATION	UNP Q8E0S7
B	52	GLY	SER	ENGINEERED MUTATION	UNP Q8E0S7
B	184	ALA	CYS	ENGINEERED MUTATION	UNP Q8E0S7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	19	Total O 19 19	0	0
2	B	15	Total O 15 15	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.48Å 49.42Å 52.71Å 87.86° 70.47° 89.40°	Depositor
Resolution (Å)	25.00 – 2.30 34.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (25.00-2.30) 94.8 (34.40-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.247 , 0.304 0.247 , 0.291	Depositor DCC
$R_{free}$ test set	904 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.8	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.014 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2983	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.92	2/1521 (0.1%)	0.82	1/2063 (0.0%)
1	B	0.80	1/1476 (0.1%)	0.88	4/2001 (0.2%)
All	All	0.86	3/2997 (0.1%)	0.85	5/4064 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	TYR	CD1-CE1	-6.59	1.29	1.39
1	A	63	TYR	CD2-CE2	-6.48	1.29	1.39
1	B	143	PHE	CD1-CE1	5.44	1.50	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	ALA	CB-CA-C	6.33	119.60	110.10
1	B	126	PRO	N-CA-CB	6.04	110.55	103.30
1	A	121	ALA	CB-CA-C	5.55	118.42	110.10
1	B	187	TYR	CB-CA-C	5.25	120.89	110.40
1	B	177	ASP	CB-CG-OD1	5.16	122.94	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1495	0	1516	66	0
1	B	1454	0	1465	49	0
2	A	19	0	0	2	0
2	B	15	0	0	0	0
All	All	2983	0	2981	114	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 114 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:THR:OG1	1:B:186:PRO:HA	1.35	1.25
1:A:129:LYS:O	1:A:132:THR:HG23	1.50	1.11
1:A:123:ARG:O	1:A:123:ARG:HG3	1.49	1.10
1:B:186:PRO:HD2	1:B:189:ILE:HG21	1.30	1.10
1:A:76:VAL:HG13	1:A:87:ILE:HD11	1.38	1.02

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	187/230 (81%)	173 (92%)	14 (8%)	0	100	100
1	B	182/230 (79%)	173 (95%)	8 (4%)	1 (0%)	32	39
All	All	369/460 (80%)	346 (94%)	22 (6%)	1 (0%)	44	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	205	GLU



### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	158/191 (83%)	149 (94%)	9 (6%)	24	32
1	B	151/191 (79%)	135 (89%)	16 (11%)	8	9
All	All	309/382 (81%)	284 (92%)	25 (8%)	14	17

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	65	ARG
1	B	68	GLU
1	B	189	ILE
1	B	67	LEU
1	B	94	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	B	155	GLN
1	B	97	GLN
1	A	155	GLN
1	B	147	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	191/230 (83%)	0.55	18 (9%)	9 12	18, 37, 69, 85	0
1	B	188/230 (81%)	1.07	35 (18%)	1 2	21, 45, 84, 103	0
All	All	379/460 (82%)	0.81	53 (13%)	3 5	18, 41, 78, 103	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	PRO	9.1
1	B	188	MET	8.0
1	B	207	THR	7.6
1	A	60	VAL	7.4
1	A	44	TYR	6.6

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.